Status Report on the Component Models Developed in the Modelica Framework: Reverse Osmosis Desalination Plant & Thermal Energy Storage

Jong Suk Kim Konor Frick (INL & NC State University) May 2018



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May 2018

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Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

ABSTRACT

This report has been prepared as part of an effort to design and build a Modeling and Simulation (M&S) framework to assess the economic viability of a Nuclear-Renewable Hybrid Energy System (N-R HES). In order to facilitate dynamic M&S of such an integrated system, research groups in multiple national laboratories and universities have been developing various subsystems as dynamic physics-based components using the Modelica programming language. In Fiscal Years (FYs) 2015, Idaho National Laboratory (INL) performed a dynamic analysis of two region-specific N-R HES configurations, including the gas-to-liquid (natural gas to Fischer-Tropsch synthetic fuel) and brackish water Reverse Osmosis (RO) desalination plants as industrial processes. In FYs 2016–2017, INL developed two additional subsystems in the Modelica framework: (1) a high-temperature steam electrolysis plant as a high priority industrial plant to be integrated with a light water reactor within an N-R HES and (2) a gas turbine power plant as a secondary energy supply.

In FY 2018, the RO desalination system model developed in FY 2015 has been updated such that the model is compatible with the most recent version of the ThermoPower library. Special attention has been given to the controller settings based on process models, aiming to improve process dynamics and controllability. A dynamic performance analysis of the updated RO desalination plant was carried out to evaluate the technical feasibility (load-following capability) of such a system operating under highly variable conditions requiring flexible output. Simulation results involving several case studies show that the suggested control scheme could maintain the controlled variables (including the variable electrical load and RO feed pressure) within desired limits under various plant operating conditions. The results also indicate that the proposed RO plant could provide operational flexibility to participate in energy management at the utility scale by dynamically optimizing the use of excess plant capacity within an N-R HES.

As an alternative to battery storage a scalable Sensible Heat Thermal Energy Storage (TES) System has been developed in the Modelica framework in FY 2018. TES is more flexible than battery storage since it can act as either an electrical peaking unit or steam production facility depending on user requirements. Further, from an economic standpoint thermal storage has a considerably longer life expectancy than even the most cutting-edge battery storage systems. The Thermal Energy Storage System implemented was adapted from an existing FORTRAN model, is fully scalable, and has been shown to be capable of storing excess energy when available and supplying peaking demand when required. Such a system will provide a load-leveling option for N-R HESs as the levels of intermittent renewables continue to increase. Simulation results show the TES system's ability to store excess power when available and provide upwards of 200 MW_e of peaking demand when needed.

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ACRONYMS

ACV Auxiliary Control Valve

BWRO Brackish Water Reverse Osmosis

DS Direct Synthesis

Dymola Dynamic Modeling Laboratory

FBV Flow Bypass Valve FCV Flow Control Valve

FOPTD First-Order-Plus-Time-Delay

FY Fiscal Year HP High-Pressure

HTSE High-Temperature Steam Electrolysis

IHX Intermediate Heat ExchangerINL Idaho National LaboratoryM&S Modeling and SimulationMGPD Million Gallons per Day

N-R HES Nuclear-Renewable Hybrid Energy System

PCV Pressure Control Valve
PI Proportional-Integral
PRV Pressure Relief Valve

PV Photovoltaic

RO Reverse Osmosis

TDS Total Dissolved Solids
TES Thermal Energy Storage
VEL Variable Electrical Load

Status Report on the Component Models Developed in the Modelica Framework: Reverse Osmosis Desalination Plant & Thermal Energy Storage

1. INTRODUCTION

The report provides the current status on component models developed in the *Modelica*¹ framework at Idaho National Laboratory (INL) under the Nuclear-Renewable Hybrid Energy System (N-R HES) program. In Fiscal Year (FY) 2015, INL identified two region-specific N-R HES configurations to be located in West Texas and Arizona for preliminary technical and operational economic analysis [1-7]. The first configuration employs a nuclear plant and a series of wind turbines to produce electricity and convert carbon resources (natural gas) to synthetic liquid fuels (gasoline and diesel) using excess thermal capacity. The second configuration employs a nuclear plant and solar Photovoltaic (PV) stations for energy generation and yields electricity to meet grid demand and to produce fresh water via Reverse Osmosis (RO) desalination using excess electrical capacity. Both systems have been implemented in the Modelica framework [8]. In FY 2016, INL developed two additional subsystem models: a High-Temperature Steam Electrolysis (HTSE) plant, which employs planar solid oxide electrolysis cells, and a gas turbine power plant [9]. In FY 2017, five new components (i.e., a feedwater pump, a multi-stage compression system, a sweep-gas turbine, flow control valves, and pressure control valves) were incorporated into the HTSE system model developed in FY 2016, aiming to more realistically characterize all key components of concern [10].

In FY 2018, the RO desalination plant (or simply referred to as the RO plant) model developed in FY 2015 was updated such that the model is compatible with the most recent version of the ThermoPower library; the Proportional-Integral (PI) controller parameters were tuned to improve the dynamic responses of the updated RO desalination system. In addition, an additional energy storage unit, i.e., a Sensible Heat Thermal Energy Storage (TES), was developed. The models were implemented using the commercially available Modelica-based Modeling and Simulation (M&S) environment, i.e., a Dynamic Modeling Laboratory (Dymola) version 2017 FD01 [11]. In-house developed packages and open-source libraries were utilized to facilitate M&S. In particular, the *Modelica standard library* version 3.2.2 [12] and *ThermoPower library* version 3.1beta.0 [13] were utilized.

The remainder of this report is organized into two sections. Section 2 presents an overview of the proposed RO plant model (including control design) and simulation results involving several case studies, followed by conclusions. Section 3 is organized in the same fashion as Section 2, but for the proposed TES model.

2. REVERSE OSMOSIS DESALINATION PLANT

Desalination is one of the solutions to bridge the gap between drinking water supply and demand. Of the various methods used for desalination, e.g., multi-stage flash, multi-effect and vapor compression distillations; electro-dialysis; and RO, RO is the predominant means of producing fresh water throughout the world.

¹ *Modelica* is an object-oriented, equation-based programming language suitable for computational applications with high complexity requiring high performance.

1

2.1 System Overview

RO desalination utilizes a semi-permeable membrane, which allows water to pass through but not salts, thus separating the fresh water from the saline feed water. A typical Brackish Water RO (BWRO) plant (see Figure 1(a)) consists of four main components: feed water pretreatment, High-Pressure (HP) pumping, membrane separation, and permeate (fresh water) post-treatment. Figure 1(b) depicts the configuration of an RO vessel (a multi-element module) used in RO desalination, which typically comprises of six to eight membrane modules connected in series. The concentrate water rejected by the first membrane module plays a role as the feed water for the second membrane module by the successive order, and so on. These pressure vessels are arranged in rows in each membrane stage, with two-stage membrane separation being typical in BWRO. Each stage has a recovery of 50–60%, achieving overall system recovery of 70–85% [7].

In this report, the modeling efforts of BWRO desalination process were focused on the two main components, i.e., HP pumping and membrane separation, enclosed in the dashed box shown in Figure 1(a); therefore, the only energy use of the process is the energy consumption by HP pumps. The BWRO plant was sized for 15.66 m³ s⁻¹ (357.4 Million Gallons per Day [MGPD]), which requires 45 MW_e of electrical power to generate the required feed (operating) pressure (16.5 barg) for desalting the brackish water, containing 3500 ppm of Total Dissolved Solids (TDS). Table 1 reports the design specifications of the proposed BWRO plant.

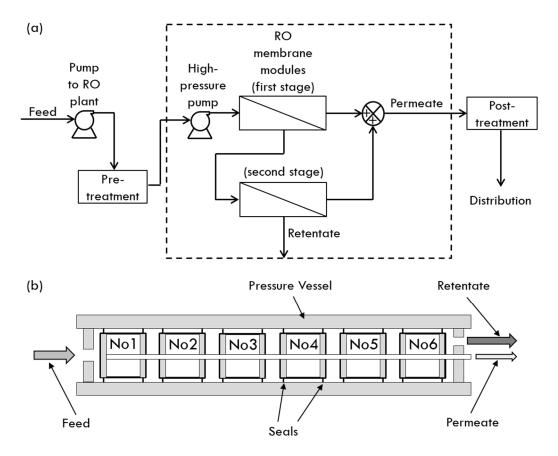


Figure 1. RO desalination: (a) process flow diagram for a two-stage BWRO plant and (b) schematic of an RO vessel, which consists of six membrane modules in series.

Table 1. BWRO plant specifications.

Symbol	Description	Unit	Value
N_{pump}	Number of HP pumps, each of which is rated at 1 MW _e	_	45
\mathcal{E}_{pump}	Pump efficiency	%	80
ω	Pump shaft rotational speed	rpm	2240
V_{op}	Valve opening of the pneumatic pressure control valve	%	80
N_{TR}	Number of RO unit trains	_	45
$N_{V\!E}$	Number of pressure vessels per one RO unit train	_	220
N_{ST}	Number of stages	_	2
N_M	Number of RO modules per one pressure vessel (or stage)	_	6
T_f	Feed temperature	°C	25
S_f	Feed salinity	ppm	3500
p_f	Feed (operating) pressure	barg	16.5
p_p	Permeate pressure	barg	0
Q_p	Permeate volumetric flow rate	$m^{3} s^{-1}$	15.66
-		[MGPD]	[357.4]
$P_{I, RO, n}$	Rated electrical load in the BWRO plant	MW_e	45
\bar{S}_{p}	Average permeate salinity (quality)	ppm	60
R_S	Salt rejection	%	99.2
R_{wI}	Water recovery in the first stage	%	48
R_{w2}	Water recovery in the second stage	%	46
R_w	Overall water recovery	%	72

Figure 2 shows the top-level Modelica model for the BWRO plant, which is compatible with the *ThermoPower library* version 3.1beta.0, implemented within the Dymola development environment.

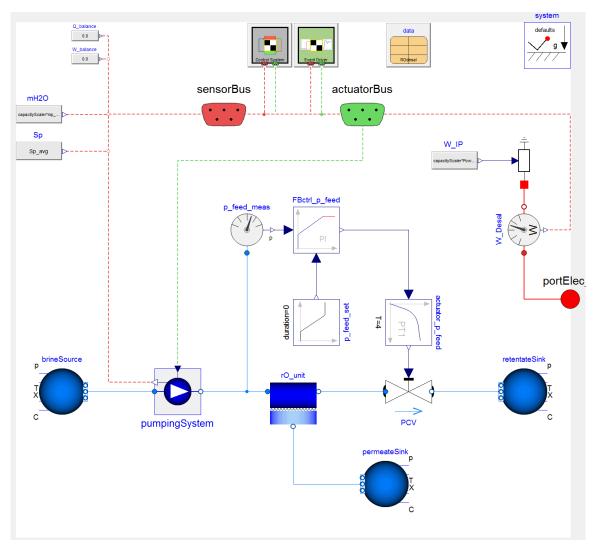


Figure 2. Top-level model for the BWRO plant implemented in Modelica.

2.2 Control System

Regulatory control strategies (single-input single-output control scheme) for a BWRO desalination system were developed (see Figure 3) to achieve two control objectives: (1) meet the power consumption requested by the system supervisor $L_{E, sp}$, i.e., Variable Electrical Load (VEL), and (2) to maintain feed (operating) pressure at the desired value (or set point) $p_{f, sp}$. While the former is met by adjusting the pump shaft rotational speed ω , the latter can be controlled by adjusting the opening of the pneumatic Pressure Control Valve (PCV) V_{op} located in the retentate stream. This control scheme ensures that the permeate quality (or salt rejection) is maintained within the desired limits, regardless of the change in the VEL requested to the desalination plant by a supervisory controller.

Among the various techniques available to determine controller feedback settings, such as Direct Synthesis (DS) method, internal model control method, controller tuning relations, and frequency response techniques, the DS method was employed to tune the PI controller settings, with the assumptions that the process models are perfect (no errors) and can be approximated by First-Order-Plus-Time-Delay

(FOPTD) models. The results are summarized in Table 2. For detailed reading on the DS method, see [14].

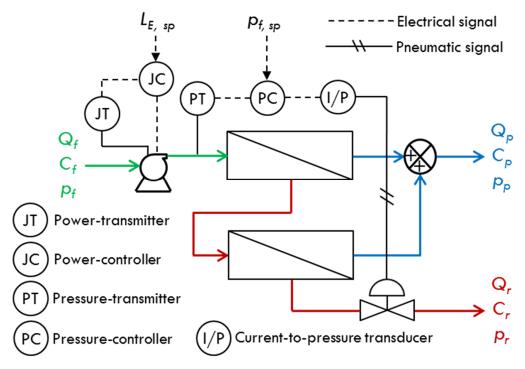


Figure 3. A control schematic of an RO unit train, with two-stage membrane separation.

Table 2. Parameters of the FOPTD model approximations and corresponding PI controller settings based on the DS method.

Symbol	Description	Value	
		VEL controller	Feed pressure controller
K	Model gain	480 (W rpm ⁻¹)	-13.2 (bar)
τ	Time constant	20 (s)	30.6 (s)
$ au_c$	Desired closed-loop time constant	6.67^{a} (s)	10.2^{a} (s)
θ	Time delay	0	0
K_c	Controller gain	0.00625 (rpm W ⁻¹)	-0.228 (bar ⁻¹)
$ au_I$	Integral time	20 (s)	30.6 (s)
y^{min}	Lower bound on controller output	600 (rpm)	0.05
y^{max}	Upper bound on controller output	3000 (rpm)	1

^a Setting $\tau_c = \tau_I/3$ means that the desired closed-loop response is three times faster than the open-loop response.

2.3 Simulations

Two case studies (Cases 1–2) were conducted to analyze the dynamic performance of the proposed BWRO plant. The key process variables (permeate flow rate and salinity; total power consumption; and

RO feed pressure, which in turn affects the quality and throughput of the fresh water produced) were observed to evaluate the technical feasibility of such a system, operating under highly flexible conditions requiring flexible output, within N-R HESs.

Renewable energy generation was modeled as a time-series input signal to the power-smoothing battery based on solar irradiance and ambient temperature data for a PV system or based on wind speed data for a wind farm [6, 7]. Historical data of solar irradiance and ambient temperature at Southwest Solar Research Park in Phoenix, Arizona² and that of wind speed measured in West Texas³ were obtained from the National Renewable Energy Laboratory database and used in the case studies. For the mathematical models and the values of model parameters used to calculate PV solar and wind powers in this report, see [4].

2.3.1 Case 1: Load-following responses with PV solar power

In Case 1, the load-following capability of the proposed BWRO plant as a flexible load resource under variable PV solar power generation was demonstrated. Figure 4 shows the time series of the key process variables simulated for one week in response to changes in the VEL (i.e., PV solar power plus a constant minimum load [15 MW_e]) delivered to the plant. As seen in Figure 4(a), the RO plant could effectively absorb local and instantaneous variability in the renewable power source by changing the $L_{E, sp}$ accordingly. Notice from Figure 4(c) and Figure 4(d) that while the production (Q_p) and concentration (S_p) of fresh water varied as the demand $(L_{E, sp})$ varied, the salinity of the fresh water produced was less than a drinking water taste threshold set by U.S. Environmental Protection Agency [15] (i.e., TDS of 500 ppm), ensuring acceptable salt rejection rates over the entire range of RO operating conditions. This was achieved by adequately maintaining the p_f near its desired set point regardless of the VEL diverted to the RO plant (see Figure 4(b)). These results suggest that the N-R HES, with a high penetration of PV generation, can act as a highly responsive device to meet load-following needs by accordingly delivering the necessary electricity generation profile demanded by the electric grid, while correspondingly adjusting itself to maintain adequate operating conditions. Moreover, since an RO plant can be operated at its minimum turndown for as long as requested, the N-R HES configuration including the RO plant can maintain the change in its electrical production for a sufficient duration.

² Accessed on May 12, 2018 at http://www.nrel.gov/midc/ssrp/

³ Accessed on May 14, 2018 at http://www.nrel.gov/grid/wind-integration-data.html

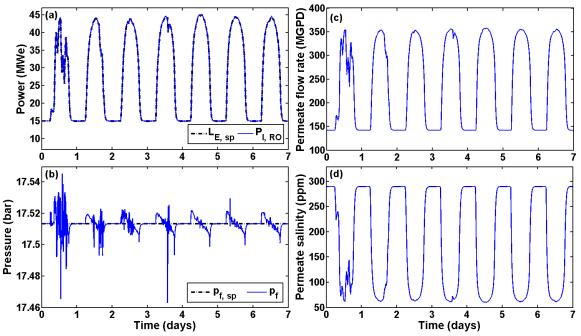


Figure 4. Output responses to the VEL for Case 1: (a) $L_{E, sp}$ vs. $P_{I, RO}$, (b) $p_{f, sp}$ vs. p_{f} , (c) Q_{p} , and (d) S_{p} . The subscript sp denotes the set point.

2.3.2 Case 2: Load-following responses with wind power

This test was designed to assess the capability of the same system considered in Case 1 for load following, but in coordination with wind power generation. The results simulated for one week are plotted in Figure 5. Similar to the results shown in Case 1, the variability introduced by the renewable (wind) source was essentially accommodated by the use of the flexible electrical load provided by the RO plant. As it can be seen, the RO system could closely track the time-varying electrical load (Figure 5(a)) requested by the system supervisor for freshwater production (Figure 5(c)), while maintaining the desired RO feed pressure (Figure 5(b)) and permeate quality (Figure 5(d)) at all times.

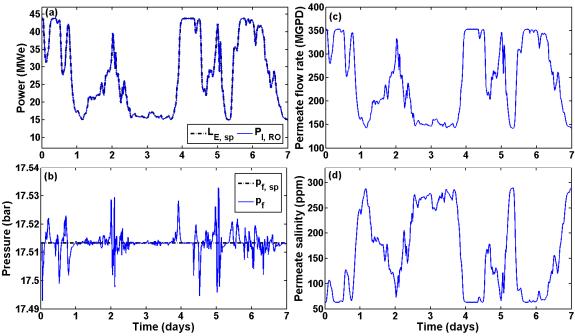


Figure 5. Output responses to the VEL for Case 2: (a) $L_{E, sp}$ vs. $P_{I, RO}$, (b) $p_{f, sp}$ vs. p_{f} , (c) Q_{p} , and (d) S_{p} . The subscript sp denotes the set point.

2.4 Conclusions – Reverse Osmosis Desalination Plant

The M&S framework to assess the economic viability of an N-R HES is reaching the maturity level necessary to begin analysis of realistic cases. In particular, the FY 2015 Modelica model developed for integration of the RO process with a nuclear reactor has been updated such that the model is compatible with the most recent version of the ThermoPower library. In addition, the control parameters have been tuned based on process models.

A dynamic performance analysis of the updated RO desalination plant was carried out to evaluate the technical feasibility of such a system operating under highly variable conditions requiring flexible output. Simulation results show that the suggested control scheme can maintain the controlled variables within desired limits under various plant operating conditions. The analysis also shows that the proposed RO plant, when integrated within an N-R HES, can respond quickly and maintain the required change for a sufficient duration in response to large, rapid net demand variations. Its operational flexibility and the variety of potential N-R HES configurations in which it can be integrated make the RO process a good candidate for integration from a technical point of view.

3. THERMAL ENERGY STORAGE

Sensible heat storage involves the heating of a solid or liquid without phase change and can be deconstructed into two operating modes: charging and discharging. A two-tank TES system is a common configuration for liquid sensible heat systems. In the charging mode cold fluid is pumped from a cold tank through an Intermediate Heat Exchanger (IHX), heated, and stored in a hot tank while the opposite occurs in the discharge mode. Such systems have been successfully demonstrated in the solar energy field as a load management strategy [16].

3.1 System Overview

The configuration of the TES system is shown in Figure 6. An outer loop interfaces with the reactor's balance of plant directly through four parallel auxiliary turbine bypass valves connected at the pressure equalization header, each staged to open at a certain percent of the maximum auxiliary flow demand. Bypass steam is directed through an IHX and ultimately discharged to the main condenser. An inner loop containing a TES fluid consists of two large storage tanks along with several pumps to transport the TES fluid between the tanks, the IHX and a steam generator. Flow Bypass Valves (FBVs) are included in the discharge lines of both the "hot" and "cold" tanks to prevent deadheading the pumps when the Flow Control Valves (FCVs) are closed. Therminol-66 is chosen as the TES fluid in this work as it is readily available, can be pumped at low temperatures, and offers thermal stability over the range (-3°C-343°C) which covers the anticipated operating range of the TES system (203°C-260°C). Molten salts (e.g. 48% NaNO₃ – 52% KNO₃) were not considered, as the anticipated operating temperatures fall below their 222°C freezing temperature [17]. The TES system is designed to allow the reactor to run continuously at ~100% power over a wide range of operating conditions. During periods of excess capacity, bypass steam is directed to the TES unit through the auxiliary bypass valves where it condenses on the shell side of the IHX. TES fluid is pumped from the cold tank to the hot tank through the tube side of the IHX at a rate sufficient to raise the temperature of the TES fluid to some set point. The TES fluid is then stored in the hot tank at constant temperature. Condensate is collected in a hot well below the IHX and drains back to the main condenser or can be used for some other low pressure application such as chilled water production, desalination or feed-water heating. The system is discharged during periods of peak demand, or when process steam is desired, by pumping the TES fluid from the hot tank through a boiler (steam generator) to the cold tank. This process steam can then be reintroduced into the power conversion cycle for electricity production or directed to some other application through the PCV. A nitrogen cover gas dictates the tank pressures during charging and discharging operation. Should a more in-depth analysis of the thermal energy storage system be desired a more detailed, and computationally expensive, model has been designed by Frick [18]. However, the level of detail presented in this reference would make its integration with the current Modelica framework prohibitive and unnecessary for the calculations desired.

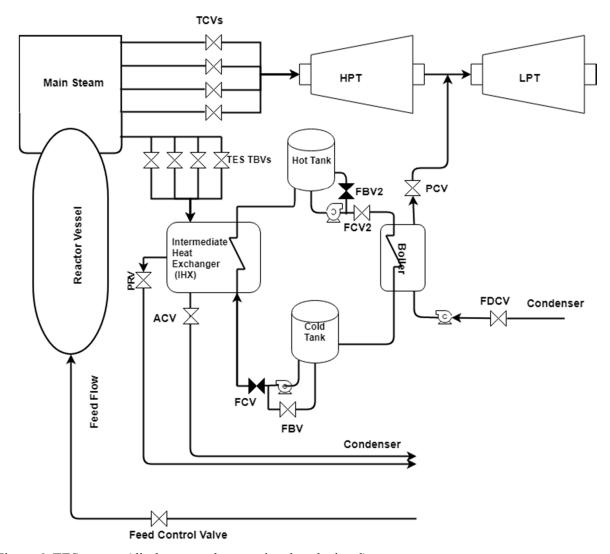


Figure 6. TES system (discharge mode operational as depicted).

3.2 Control System

There are two modes of operation present in the sensible heat thermal energy storage system: charging and discharging. In the charging mode cold fluid is pumped from a cold tank through an IHX, heated, and stored in a hot tank while the opposite occurs in the discharge mode.

3.2.1 Charging mode control

The TES system has four sets of valves used to control system parameters: auxiliary bypass valves, the TES FCV, the Auxiliary Control Valve (ACV), and Pressure Relief Valves (PRVs).

The goal of the bypass flow controller is to provide bypass steam to the TES system at a rate sufficient to maintain the reactor at or near its nominal steady state value. The bypass valve controller generates an error signal based on the difference between measured bypass flow and a bypass flow demand signal. The bypass demand signal assumes the required bypass flow is proportional to the relative difference between the nominal full power turbine output and the instantaneous electric load.

Flow from the cold tank to the hot tank is via a TES flow control valve. The TES flow control valve operates using a three-element controller, where the first error signal is designed to maintain the TES fluid temperature leaving the IHX at some reference value. The second error signal is designed to roughly match the heat input into the TES fluid with the heat bypassed to the IHX.

The ACV maintains IHX hot well level. This valve operates on a three-element controller based on the level of the IHX and the difference in mass flows into and out of the IHX. Gains were selected to allow for smooth operation of the ACV over foreseeable operating bands.

PRVs have been installed in the IHX to mitigate pressure increases. Should pressure reach an upper set point the valves will open and will not close until the pressure falls below a lower set point.

The only parameters directly controlled during charging mode operation of the TES system are the IHX exit temperature on the inner loop and the level in the IHX. All other variables including IHX pressure, tank levels, inner loop mass flow rate, and heat transfer across the IHX are determined from the mass, energy and momentum balances on the system.

A stop valve (not shown in Figure 6) is placed in the flow line between the cold tank and hot tank to ensure tank pressure and level stay below designated set points. Should either the pressure or level set points be exceeded the stop valve will close and TES fluid flow between the tanks will cease. A redundant control on level is that the volume of TES fluid in the system is less than the total volume of either tank

3.2.2 Discharging mode control

Alternatively, during times of excess demand the system will be discharged. The discharge mode can be operated in two different modes. It can operate either as an electrical peaking unit to supplement the electric grid during times of high demand, or it can be used as a source of steam for ancillary industrial applications. Both modes have been designed, each with its own set of control algorithms. Note that the steam peaking simulation is not shown here because the ability to use this in the currently installed cash flow optimizer is limited.

Electrical Peaking Unit

The electrical peaking unit control strategy assumes three control valves. A PCV in the boiler to maintain pressure control, a Feed Control Valve to allow for level control within the boiler and an FCV on the tube side of the steam generator to regulate the amount of TES flow from the hot tank to the cold tank. Feed control is based on a standard three element controller where the error signals are level and steam flow/feed flow mismatch. The TES flow control valve modulates to match turbine output with turbine demand.

Steam Peaking Unit

The electrical peaking unit control strategy assumes three control valves. A PCV in the boiler to maintain pressure control, a Feed Control Valve to allow for level control within the boiler and an FCV on the tube side of the steam generator to regulate the amount of TES flow from the hot tank to the cold tank. Feed control is based on a standard three element controller where the error signals are level and steam flow/feed flow mismatch. The TES flow control modulates to match steam flow out of the boiler with steam demand.

3.3 Simulations

To illustrate the storage capabilities inherent with the sensible heat thermal energy storage system a demand profile was constructed with the intent of taxing the TES system's storage capabilities. More realistic dispatch cycles will be less demanding since it is unrealistic to imagine turbine demand swings

upwards of 400 MW_e over 2 or 3 hour cycles. Instead these simulations are intended to show the inherent stability intrinsic to storage units of this nature.

Table 3. TES parameters for simulation.

Parameter	Value
TES Fluid	Therminol-66
Reactor Size Assumed	3400MW _{th} (~1000 MW _e) 4-loop PWR
Nominal Full Power Reactor Steam Flow	$6.895 \times 10^6 \text{ kg/hr} (15.2 \times 10^6 \text{ lbm/hr})$
Maximum TES Steam Accommodation	~20% nominal steam flow
Hot Tank Volume	226,535 m ³
Cold Tank Volume	226,535 m ³
Boiler Operational Pressure	1.379 MPa (200 psia)
IHX and Boiler Tube Material	Inconel-610
LPT Re-entrance Pressure	1.207 MPa (175 psia)

The simulation results are presented in Figure 7(a)–(c). Parameters used for the given simulation are seen in Table 3. Figure 7(a) shows the demand ranging from a minimum demand of 80% nominal turbine output to 120% nominal turbine output. This corresponds to excess capacity of 200 MW $_{\rm e}$ and subsequently a peaking demand of 200 MW $_{\rm e}$. As previously mentioned when net demand is greater than 100% the TES system is required to make up for this extra demand by discharging TES fluid through the boiler to allow operation as a peaking unit. Alternatively, a net demand less than 100% corresponds to the TES system being charged as the excess energy is dumped into the IHX as opposed to being pushed through the main turbine system.

Figure 7(b) demonstrates the TES system capability to match the turbine demand throughout the full 26 hour simulation. Of note is that a tank capacity of 226,535 m³ of Therminol-66 is sufficient to withstand full discharge for 3-4 hours when the hot tank is nearly full to begin with. The proper amount of TES-fluid one should place in the tanks will be directly linked to the predicted storage needs for a given region.

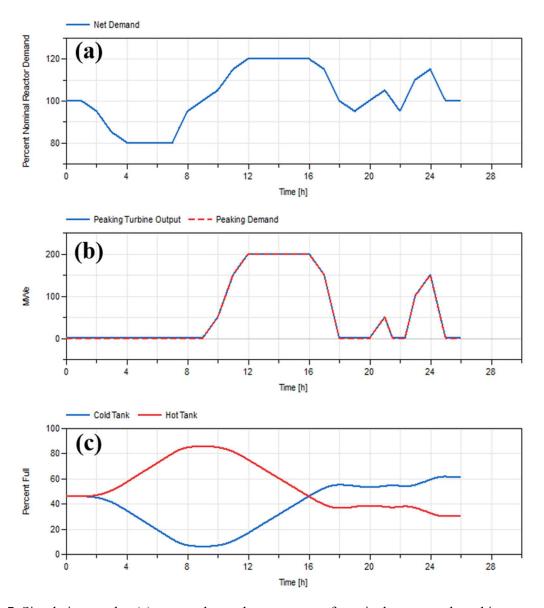


Figure 7. Simulation results: (a) system demand as a percent of nominal reactor only turbine output, (b) peaking unit demand, and (c) TES system tank levels.

3.4 Conclusions - Thermal Energy Storage

The results presented demonstrate the TES system is capable of storing massive quantities of thermal energy and is able to then reintroduce this energy to produce electricity when required. With the implementation of a TES system, decreases in capacity factor and increased stresses on reactor plant components can be minimized, improving economic return over the lifespan of the reactor. It should be noted the optimal size TES system will be region and configuration dependent.

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